

Bipolar spin filter in a quantum dot molecule

F. Mireles, E. Cota, and F. Rojas

*Departamento de Física Teórica, Centro de Ciencias de la Materia Condensada –
Universidad Nacional Autónoma de México, Ensenada, Baja California, México 22800*

S. E. Ulloa

*Department of Physics and Astronomy and Nanoscale and Quantum
Phenomena Institute, Ohio University, Athens, OH 45701-2979*

We show that the tunable hybridization between two lateral quantum dots connected to non-magnetic current leads in a ‘hanging-dot’ configuration that can be used to implement a bipolar spin filter. The competition between Zeeman, exchange interaction, and interdot tunneling (molecular hybridization) yields a singlet-triplet transition of the double dot *ground state* that allows spin filtering in Coulomb blockade experiments. Its generic nature should make it broadly useful as a robust bidirectional spin polarizer.

Controlling the spin of electrons in mesoscopic systems is an important task in ‘spintronic devices,’ as well as in the fundamental understanding of spin relaxation and coherence.¹ Experiments using diluted magnetic semiconductors (DMS) heterostructures have reported excellent polarization values ($\sim 90\%$).² Spin-polarized currents have been observed using ferromagnetic leads in semiconductor quantum dots.³ Pioneering studies have also appeared recently where different spin-filter and polarization measurements have been described where no polarization of the leads is needed. The original proposal of Recher *et al.*⁴ – to produce a spin-polarized current using the Zeeman effect in a quantum dot with odd number of electrons – has been recently implemented in beautiful experiments by Hanson *et al.*⁵ They report nearly pure ($\sim 99\%$) spin collection for spin-unpolarized leads, a reflection of the large orbital energy separation achieved in their small quantum dots. Moreover, they can swiftly flip the spin polarization (a ‘bipolar’ filter) by changing the charge state of the single dot. Bidirectional spin filtering making clever use of spin coherence⁶ and magnetic focusing was reported by Potok *et al.*,^{7,8} who achieved very good spin ($\sim 70\%$) polarization at moderate applied fields ($\sim 6T$ parallel to the plane of the dot).

Spin-blockade⁹ in double quantum dots (DQD) connected in series (sequentially) and coupled via tunneling has also been studied by Johnson *et al.*¹⁰ using transport measurements and charge sensing with quantum point contacts. They observe current rectification due to the singlet-triplet spin-blockade mechanism in the DQD. Coulomb- and spin-blockade spectroscopy studies in spin sensitive experiments were also realized recently in a two-level DQD molecule.¹¹

In this letter we show theoretically that a bipolar spin filter can be implemented at moderate fields by producing a singlet-triplet transition of the DQD *ground state*. This transition is obtained solely by tuning the hybridization (hopping) between the two quantum dots in the molecule, achieved by varying the coupling via the quantum point contact connecting the dots. The DQD is connected to

non-magnetic leads via only one of the dots, in a ‘hanging dot’ configuration (Fig. 1a). It is shown that the competition between Zeeman energy and the effective ‘superexchange’ interaction results in lower energy for the *singlet* configuration for large enough interdot tunneling and even electron number. This in turns gives rise to a natural spin selectivity, fully tunable by appropriate electrical gating of the structure. The effect is shown to arise in both the linear (low bias) and non-linear regimes of transport at low temperatures.

We model the coupled DQD molecule as a single coherent system, where the quantum dots are assumed small enough so as to have only one relevant orbital energy level on each dot with gate-controlled on-site energies ϵ_i , ($i = 1, 2$). The conducting dot in the molecule (dot 2 in Fig. 1a) is weakly coupled to non-magnetic reservoirs.

The Hamiltonian of the DQD molecule is $H = H_0 + H_{int}$, where

$$H_0 = \sum_{i,\sigma} \epsilon_i c_{i,\sigma}^\dagger c_{i,\sigma} - t \sum_{i \neq j, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} \quad (1)$$

and

$$H_{int} = U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + \frac{1}{2} \left(V - \frac{J}{2} \right) \sum_{i \neq j} \hat{n}_i \hat{n}_j \\ - J \sum_{i \neq j} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2} \sum_{i,\sigma,\sigma'} \Delta_z^{(i)} c_{i,\sigma}^\dagger (\sigma_z)_{\sigma\sigma'} c_{i,\sigma'}, \quad (2)$$

where $c_{i,\sigma}^\dagger$ is the creation operator for electrons on each dot i with spin σ (\uparrow, \downarrow), t describes the interdot orbital hybridization, which can be tuned in a typical setup by voltages on the quantum point contact defining the connection between dots. In (2), U is the double occupation charging energy, V is the interdot Coulomb interaction, J gives the interdot exchange interaction (with $J > 0$)¹², and finally $\Delta_z^{(i)} = |g| \mu_B B_z^{(i)}$ is the Zeeman energy splitting for dot i in a local magnetic field $B_z^{(i)}$. Such local splitting could be produced for instance by nanoscale magnetic disks of ferromagnetic material,¹³ as suggested

recently.¹⁴ Spin-orbit coupling is also introduced as in [15] but its strength is typically small ($t_{SO} < 0.1t$), and does not appreciably affect our results and conclusions.

We are interested in the effective low-occupation of the DQD, so that the relevant basis (levels close to the Fermi energy) consists of a few states for $N = 0, 1$ and 2 electrons.

Consider now the case with symmetrical QD's ($\epsilon_1 = \epsilon_2 = \epsilon$), and homogeneous magnetic field, $\Delta_z^{(1)} = \Delta_z^{(2)} = \Delta_z$. A non-zero magnetic field breaks the spin degeneracy in the DQD. The energy spectrum for $N = 1$ is given by $E_{1,2}^{(1)} = \epsilon - t \mp \Delta_z/2$, and $E_{3,4}^{(1)} = \epsilon + t \mp \Delta_z/2$, with (non-normalized) eigenstates $|v_1\rangle = |\uparrow, 0\rangle + |0, \uparrow\rangle$, $|v_2\rangle = |\downarrow, 0\rangle + |0, \downarrow\rangle$, $|v_3\rangle = |0, \uparrow\rangle - |\uparrow, 0\rangle$, and $|v_4\rangle = |0, \downarrow\rangle - |\downarrow, 0\rangle$, respectively. For two electrons in the DQD, the magnetic field breaks the degeneracy of the triplet states $|T_o\rangle = |\uparrow, \uparrow\rangle + |\downarrow, \uparrow\rangle$, $|T_+\rangle = |\uparrow, \uparrow\rangle$ and $|T_-\rangle = |\downarrow, \downarrow\rangle$. The competition between the Zeeman energy, the exchange and the interdot hybridization strength produces a singlet-triplet transition for the ground state, as shown schematically in Fig. 1b. For a fixed (large enough) magnetic field and $t < t_c$, the ground state is the triplet $|T_+\rangle = |\uparrow, \uparrow\rangle$ with energy $E_1^{(2)}(t < t_c) = 2\epsilon + V - \Delta_z - J$, while for $t > t_c$ the ground state is the singlet configuration $|S_o\rangle = |\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle + \alpha(|\uparrow, \downarrow, 0\rangle - |0, \downarrow, \uparrow\rangle)$, where α is t -dependent, $\alpha = 4t/(U - V - J + \sqrt{16t^2 + (U - V - J)^2})$. The singlet has a field-independent energy $E_1^{(2)}(t > t_c) = 2\epsilon + \frac{1}{2}(U + V + J - \sqrt{16t^2 + (U - V - J)^2})$. The transition occurs then at $t = t_c = \frac{1}{2}\sqrt{(2J + \Delta_z)(U - V + \Delta_z + J)}$.

The conductance per spin in the low bias regime is given by^{16,17}

$$G_\sigma(T, V_g) = \frac{e^2}{k_B T} \sum_{n=1}^{N_{max}} \sum_{\alpha, \beta} \frac{\Gamma_{n\alpha\beta}^{L\sigma} \Gamma_{n\alpha\beta}^{R\sigma}}{\Gamma_{n\alpha\beta}^{L\sigma} + \Gamma_{n\alpha\beta}^{R\sigma}} P_{n,\alpha}^{eq} \times [1 - f_{FD}(E_{n,\alpha} - E_{n-1,\beta} - \mu)] \quad (3)$$

where $\Gamma_{n\alpha\beta}^{\nu\sigma} = \gamma_{\nu\sigma} S_{\alpha\beta}^{\nu\sigma}$ is the tunneling rate involving lead ν for an electron with spin σ . $\gamma_{\nu\sigma}$ measures the tunneling amplitude from/to the leads, while $S_{\alpha\beta}^{\nu\sigma} = |\langle n, \alpha | c_\sigma^\dagger | n - 1, \beta \rangle|^2$ is the spectral weight whereby the DQD goes from a quantum state β with $n - 1$ electrons to a quantum state α with n electrons (see references for details).^{16,18,19} This conductance expression assumes weak coupling to the leads and sufficiently high temperatures that one can neglect the Kondo effect due to correlations with the reservoir electrons.²⁰

The only non-zero contributions to the spectral weights involving the DQD ground state, for the $N : 0 \rightarrow 1$ transition are $S_{11}^{\nu,\uparrow} = |\langle v_1 | c_\uparrow^\dagger | 0 \rangle|^2$, while, for $N : 1 \rightarrow 2$ one gets $S_{11}^{\nu,\uparrow} = |\langle T_+ | c_\uparrow^\dagger | v_1 \rangle|^2$, for $t < t_c$, and $S_{11}^{\nu,\downarrow} = |\langle S_0 | c_\downarrow^\dagger | v_1 \rangle|^2$, for $t > t_c$. This t -dependence of the spectral weights and the non-trivial contribution of the first excited states results in spin polarized transport through the DQD for $N > 1$, as we show below.

Figure 2 shows the conductance through the DQD molecule as function of the gate voltage V_g for vari-

ous interdot tunneling (hybridization) strengths t . The Coulomb interdot energy is set here to $V = 0.24 meV$, with $\epsilon_1 = \epsilon_2 = 0.25 meV$, $U = 1 meV$,²¹ $J = 0.01 meV$ for the DQD sizes of interest,²² $\Delta_z = 0.03 meV$, and symmetrical tunneling to/from the leads $\gamma_{\nu\sigma} = \Gamma_o = 0.25 \mu eV$. At low interdot tunneling, the conductance is completely spin polarized for the transitions $N : 0 \rightarrow 1$ and $1 \rightarrow 2$ in the DQD. Since transport in this low bias regime is determined by the ground state, the spin-up polarized conductance demonstrates that the Zeeman energy dominates at these parameters and the conductance accesses the *triplet* ground state, as one would expect. However, as the interdot tunneling increases, the electrons delocalize, increasing the hybridization and making the *singlet* configuration the ground state of the DQD. Correspondingly, the second conductance peak at higher gate voltage, for the transition $N : 1 \rightarrow 2$, has a reversed spin character with respect to the first. The conductance changes from spin *up* polarization at weak coupling ($t < 0.08$) to spin *down* polarization at higher t values ($t \geq 0.12$), with a crossover point a $t_c = 0.1 meV$, where both spin conductances are nearly identical. The large interdot hybridization results in the switch of the spin polarization for the current through the DQD, resulting in a *bipolar* spin filter with high efficiency (up to $\sim 80\%$); all by just adjusting the quantum point contact between dots.

The bipolar spin filter is robust to detuning of the on-site energies $\Delta\epsilon = \epsilon_2 - \epsilon_1$. For example, while fixing ϵ_2 and varying ϵ_1 via local gates on each dot, the bipolar function is basically unaffected for $\Delta_z \geq |\Delta\epsilon|$, except for slight shifts in the overall position of the Coulomb blockade peaks (not shown). In contrast, the spin filter effect can be strongly modified by large asymmetries in the *local* Zeeman splitting. This flexibility might be useful if one controls the local effective field in the system, via magnetic disks placed in close proximity to the dots, or local gating to affect the individual-dot g -factors, for example.

We have also explored the DQD in the non-linear regime of transport. The spin dependent current is calculated by generalizing Eq. (3) of Ref. 18. Figure 3 shows the spin polarization current map ($I_\uparrow - I_\downarrow$) in the $V_{sd} - V_g$ plane, where V_{sd} is the source-drain bias. Panel (a) shows a net electron spin current through the DQD for relatively large tunneling strength, $t = 0.15 meV$, whereas lower panel (b) depicts the case of weak tunneling, $t = 0.01 meV$. In both cases the first electron traverses the molecule with spin up (red region, indicated by an up arrow), given the spin-polarized nature of the ground state, for a range of V_{sd} until the first excited state enters the conducting window and the spin polarization is reduced (blue region). At a given V_{sd} value, increasing V_g results then in a drop in the spin polarization, with possible alternations in value (as in panel (a)). A larger interdot coupling t results in a larger $N = 1$ Coulomb diamond, as the 'bonding-antibonding' gap increases. The width of spin-up polarized current 'bands,'

for the $N : 0 \rightarrow 1$ transition (red regions), is given by Δ_z , as we would expect. Also, the separation between these bands for either fixed V_g or V_{sd} is simply $2t$. For the spin-down polarized current, this width is approximately Δ_z , as one can verify from the energy expressions above.

For small t values, as in panel (b), successive bands of polarized current are either up or near zero polarization, indicative of the predominant triplet states at or near the ground state. On the other hand, for $t > t_c$, as in panel (a), increasing V_g results eventually in a band of down-polarized current (yellow region, indicated by a down arrow), which extends over a large region in the $V_{sd} - V_g$ plane. In this regime the ground state is given

by the singlet, the result of the increased hybridization of the DQD molecular state.

Although our calculations here are for the first few electrons in the DQD molecule, our discussion should be valid for any relatively isolated manifold of the molecule level structure. In other words, low-lying states have zero spin (typical of any closed shell), and only states near the Fermi level would mix/hybridize, reproducing the regime we discuss here.

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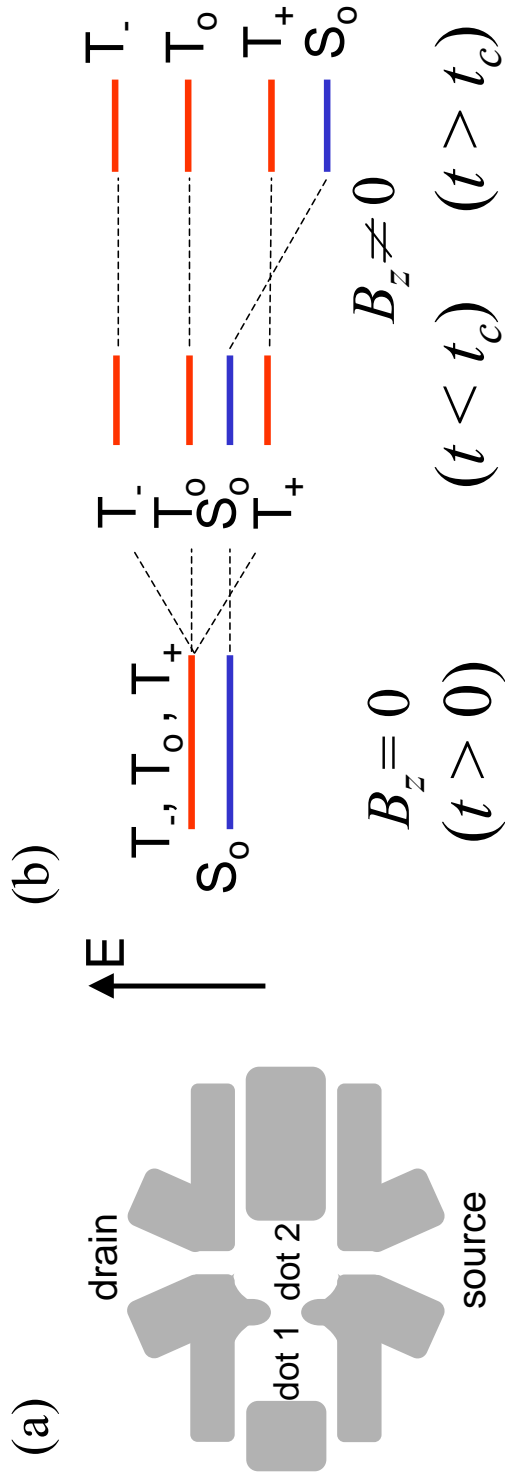


FIG. 1: (Color online) (a) Schematic of the double quantum dot structure. Current passes ‘only through’ dot 2; dots are connected via a gated quantum point contact with tunneling t . (b) Low energy level structure for two electrons in a DQD in various regimes. Notice singlet is the ground state for $t > t_c$, as shown on right.

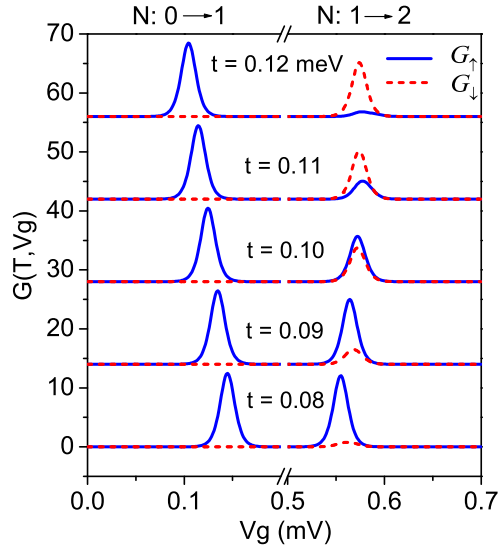


FIG. 2: (Color online) Spin-resolved conductance (in arb. units) for up (blue solid) and down (red dashed) electrons, as function of the interdot hopping amplitude t in a magnetic field. Notice that for $t > t_c = 0.1 \text{ meV}$, the second (higher V_g) Coulomb blockade conductance peak changes to spin-down, while the first Coulomb blockade peak is always spin-up. This is the bipolar filter effect. Here, $t_{SO} = 0.1t$.

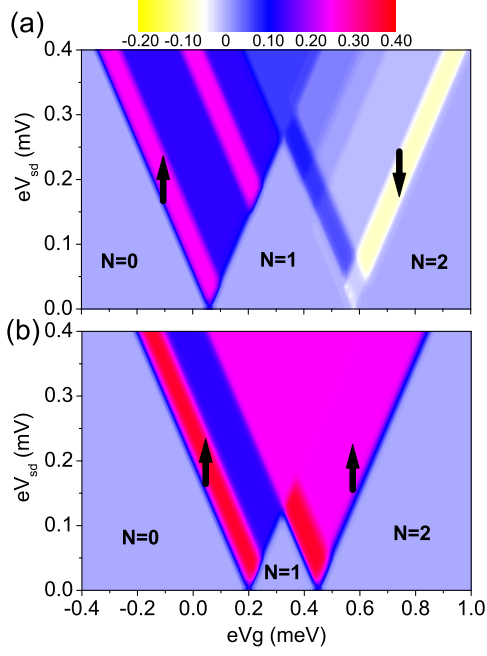


FIG. 3: (Color online) Map of the current spin polarization ($I_\uparrow - I_\downarrow$) through a DQD molecule conducting through a single dot; Zeeman splitting $\Delta_z = 0.08 \text{ meV}$. (a) Results for $t = 0.15 \text{ meV} > t_c$. Notice both bands of up (red, up arrow) and down (yellow, down arrow) spin. (b) For small interdot coupling, $t = 0.01 \text{ meV}$, only up spins dominate the current at all bias and gate conditions. Other parameters as in Fig. 2.